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#### PRELIMINARY GEOCHEMICAL GEOPHYSICAL MODEL OF YUCCA MOUNTAIN

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#### **ABSTRACT**

As part of the Nevada Nuclear Waste Storage Investigations (NNWSI) Project, a comprehensive geochemical geophysical model is being compiled. This model incorporates the current and relevant stratigraphic, petrologic, hydrogeologic, geochemical, and material data associated with a candidate repository at Yucca Mountain, Nevada. A geochemical/geophysical model is needed to (1) provide support and confidence to the Systems Performance calculations, (2) determine whether the data collected as part of the site characterization provide the information needed by the design and performance assessment task, and (3) provide the most accurate and referenced foundation on which to base the radionuclide transport calculations. In this report the known repository data are compiled and unknown parameter values are estimated based on the available data. It is concluded that more data are needed before the geochemical geophysical model of Yucca Mountain can be regarded as satisfactory and a suitable base for multidimensional predictive flow and transport simulations. Recommendations for future studies concerning site characterization and data aquisition are presented.

#### INTRODUCTION

The Nevada Nuclear Waste Storage Investigations (NNWSI) Project is charged with studying the feasibility of placing a high-level nuclear waste repository in the volcanic tuffs beneath Yucca Mountain, Nevada. The cumulative release of radionuclides to the accessible environment for 10,000 yr after disposal is limited by the Environmental Protection Agency (EPA) in conformance with 40 CFR 191 [1]. An effort is under way to collect the necessary parameter values, compile them into a geochemical geophysical model, and determine areas in which more information is required in order to (1) provide support and confidence to the Systems Performance calculations as required by issues 1.1 and 1.6 [2], (2) determine whether the data collected as part of site characterization provide the information needed by the design and performance assessment tasks, and (3) provide the most accurate and referenced foundation on which to base the radionuclide transport calculations. In this paper, a comprehensive, referenced geochemical geophysical model containing the current geochemical, stratigraphic, petrologic, hydrogeologic, material data, and source terms for the Yucca Mountain site is presented. In a recent report [3], the geochemical geophysical model described in this pager was used as a basis for a set of transport calculations known repository data are presented and unknown parameter values have been estimated based on the available data. Recommendations for future studies concerning site characterization and data aquisition are presented.

The geochemical properties and processes that affect transport are sorption and temperature. Stratigraphy, hydrogeology, material properties, and temperature are the geophysical properties and processes that are considered in the current model. The material properties and processes that are significant with respect to transport calculations are saturation, porosity, matrix tulk density, mechanical dispersion, constrictivity, and molecular diffusion [4]. As site characterization proceeds, this model will be continually updated and revised to reflect the most currently gathered information and data

are impermeable and fractured, while the nonwelded tuffs are permeable and unfractured [12]. The geologic, hydrogeologic, and geochemical properties may differ from one unit to the next. These differences may significantly impact the results of transport calculations.

Figure 1 shows in a schematic form the general stratigraphy of Yucca Mountain [5]. The stratigraphy for the model is derived from the projected base unit elevations provided by data from the TUFF Data Base [13] for the point approximately midway between the drill holes USW H-5 and USW G-4 [6]. This location was selected because smaller relative error estimates associated with the elevations were given by kriging the data obtained form drill hole data [14]. The kriging done by Campbell [14] has the advantage of connecting a measure of confidence to the elevation data. The actual elevation were taken from the TUFF Data Base [13] because the data base is very easy to access. In this case, the TUFF Data Base provides the same values for the elevations as those obtained by kriging [14]. The static water level (SWL) is defined to be at an elevation of zero meters and the bottom of the potential repository slab is at an elevation of 257.7 m.

The mountain is divided into nine fundamental units [6]: (1) Tiva Canyon welded, TCw: (2) Paintbrush nonwelded, PTn: (3) Frow Pass welded, PPw: (6) Upper Crater Flat monwelded, CFUn; (7) Bullfrog welded, BFw; (8) Middle Crater Flat nonwelded, CFMn; and (9) Tram welded, TRW. Three of the units. the Topopah Spring welded, Calico Hills nonwelded, and Middle Crater Flat nonwelded, are subdivided. The Topopah Spring welded unit is divided into three subunits, TSw1, TSw2, and TSw3. The Calico Hills nonwelded unit is broken into four subunits. Three basic subunits defined within the Calico Hills unit are CHn1, CHn2, and CHn3. A zeolitic layer intersects both CHn1 and CHn2 at points within the potential repository slab. Because the zeolitic layer is primarily within the CHn2 subunit, the first Calico Hills subunit was further divided into two smaller units. The first subdivision of CHn1, CHn1v, is a vitric layer. CHn1z is the zeolitic layer beneath CHn1v, The next two subunits, CHn2 and CHn3, are both assumed to be zeolitic layers having distinct material properties. Finally, the Middle Crater Flat unit was subdivided into three zones, CFMn1, CFMn2, and CFMn3. Each of the 16 material units are assigned values for the properties and parameters needed for transport calculations.

A zeolitic zone occurs in part of the top layer of the Calico Hills unit. This zeolitic layer is fairly a ep in the west and south of the repository block [6] but runs closer to the top of the Calico Hills unit as one moves north and east. This layer does not run through the entire mountain and would be a factor in transport calculations for only a portion of the repository. The stratigraphy of the potential repository site exhibits a large spatial variation in horizontal as well as vertical extent. The thickness of the various layers, and in cases the existence of those layers, is dependent on the location within the mountain.

# Hydrogeology

Fluid flow at Yucca Mountain occurs through heterogeneous, anisotropic, fractured tuff. Little is know about the group dwater flow in the unsaturated zone, and investigations in this area are in the preliminary stages [15,16]. Analysis Indicate that the vertical percolation is nonuniform in the unsaturated zone [15]. Fraliminary calculations [16] indicate that because of the dip of the stratigraphic units and their hydraulic properties, a significant proportion of the flow near the proposed repository horizon may be diverted laterally into a permeable fault zone. The magnitude and location of the calculated lateral flow depend upon whether matrix-flow or fracture-flow conditions are assumed for the highly fractured units, upon the flux specified at the ground surface, and upon the nydraulic properties assigned to the fault zone. The results of these calculations are further controlled

by poorly know hydraulic parameters such as the characteristic curves of moisture retention and relative permeabilities  $[\cdot 6]$ .

Although stratigraphic analyses show the presence of tipped beds, and early hydrologic studies indicate that the tipping may affect fluid flow, too little is known about these effects to incorporate them into our model at present. In this report it is assumed that the recharge rate is applied as a constant vertical velocity field over the entire mountain; this is the simplest-case scenario for simulating radionuclide transport. As site characterization proceeds, the hydrogeologic model will be updated. For all the stratigraphic units, the flow is presumed to be matrix dominated, with insignificant lateral or fracture flow. An expected value for up the average vertical flow rate, is 0.5 mm yr, whereas an extreme value may be as high as 4.5 mm yr [15,17].

## Molecular Diffusion

Molecular diffusion causes mixing of the contaminants in the fluid because each solute has its own patchine with respect to the flow comain as well as its owr velocity along that pathline. The transport time between points of interest will be lengthered if the flow velocity is relatively small so that enough time exists for a portion of the radionuclide to diffuse into the surrounding matrix fluid. Diffusion coefficients are hard to obtain, and it appears that they are not known for many of the radionuclides. For most of the actinides, the value of the diffusion coefficient changes as a function of speciation, and the speciation, both temporally and/or spatially, is generally unknown. Plutonium, because of its tendency to form colloidal structures, may have diffusivities several orders of magnitude smaller than an expected value of  $1.46 \times 10^{-5} \text{ cm}^2/\text{s}$  [18]. Therefore, since so few data were available, a single value of  $1.5 \times 10^{-5} \text{ cm}^2/\text{s}$  [18] was chosen as the diffusion coefficient for all the radionuclides. This is consistent with values for other materials, which normally have diffusion coefficients on the order of  $10^{-5}$  cm<sup>2</sup> s [19]. Actual values will be incorporated into the model as they become available.

## Constrictivity

Constrictivity,  $\tau$ , is a combination of two factors: the deviation of the pathline of transport from a straight path (the standard definition of tortuosity) and the narrowing of the pores (the standard definition of constrictivity). For actual perous systems, it is difficult to separate the two factors [20]. It is also this combined quantity that is determined experimentally. Hence, constrictivity is considered to be the combination of pathline deviation and pore narrowing. Values for  $\tau$  were determined from diffusion cell experiments [18]. For the welded units,  $\tau_{\rm c} = 0.037$ , and for the nonwelded units,  $\tau_{\rm c} = 0.030$  [18].

The available data were obtained using samples from each of the layers around and below the potential repository slab, the Topopah Spring and Calico Hills units. The data from the Topopan Spring units showed to scale effect based on sample thickness, and the value obtained from the samples within this unit was used for all of the other welded units. The Calico Hills data exhibited a very strong dependence on sample thickness, with a correlation coefficient of -0.9976 between the constrictivity coefficient and sample thickness. The anisotropic rature of the welded tuffs is potentially responsible for the scale dependence. Thus, when samples are small, there is a preferred direction for flow because of the manner in which the tuffs were formed. The experimental data were taken from samples taken with the same orientation to the tuff beds, and rence they all show the same preferchtial pattern to flow [18]. It is believed that this dependence will cease to exist after a certain sample size is exceeded [18]. Thus, the asymptotic value should be used for the Calico Hills unit as well as the other non-eleded

units, recause all the material layers have thicknesses that are greater than any of the samples used in the experiments.

# Material Properties

The properties and characteristics of the geologic media that affect transport are saturation, porosity, matrix bulk density, and dispersivity. The matrix bulk density affects transport only through the geochemical process and the particular definition of equilibrium sorption used in this report. Based on the best available information, we have assigned values for these properties to the 16 subunits. Values for saturation ( $\sigma$ ), porosity ( $\varepsilon$ ), and matrix bulk density ( $\sigma$ ) for the 15 subunits are given in Table II. These values are the unweighted means of drill hole data provided by the TUFF Data Base [12,21]. Note that the porosities of the Topopah Spring units are a factor of three less than the porosities of the Calico Hills norwelded units.

Mechanical dispersion is the mixing process that occurs when streamlines converge in the narrow necks between particles and diverge in the large interstices. Information concerning mechanical dispersion and dispersivity does not exist at this time. One estimate of the dispersion coefficient for the tuff is 1.0 x 10<sup>-3</sup> cm<sup>2</sup> s [22]. Since the longitudinal dispersion coefficient controls the amount of dispersion in the direction of flow, which is a major factor in the transport of radionuclides, a need exists to determine this quantity with more confidence. Also, the values currently being used are the same for both the highly fractured, welded units and the relatively unfractured, nonwelded units. The highly fractured units should exhibit a larger value of dispersivity than do the nonwelded units. Where there are large differences in the degree of fracturing the values may differ by more than a factor of 10. The field tracer experiments to be conducted at the C-Wells will provide more data on dispersion in Yucca Mountain tuffs.

#### Temperature

The density of water at 3.98°C is 1.0000 g/cm<sup>3</sup>. Since the ambient temperature within Yucca Mountain is estimated at 34°C, the appropriate density for water is 0.99440 g/cm<sup>3</sup> [23]. This change is relatively insignificant when compared with the uncertainties of other parameters, such as matrix density or saturation. The viscosity of water at 20°C is 0.01002 g/(s-cm). At 34°C, the viscosity of water is 0.00734 g s-cm, resulting in a 27% decrease in value [23]. The viscosity is used in the flow calculations. The viscosity is not required for transport calculations if the flow field is predetermined.

## RADIONUCLIDE SOURCE

For transport calculations, the initial concentrations of the radionuclides must be known. For uranium,  $5.0 \times 10^{-6} \, \mathrm{g~cm}^3$  (derived from an original value of 5 ppm on a mass basis [24]) is assumed to be released from the waste parkage. For technetium,  $2.6 \times 10^{-6} \, \mathrm{g~cm}^3$  was calculated from the 450 pCi cm obtained for solutions over H. B. Robinson bare fuel [24]. The conversion factor used in the technetium calculation is  $5.87 \times 10^{-6} \, \mathrm{gg~pCi}$ . This is not the expected long-term source value; rather it is the early preferential release value [24]. Long-term technetium release would be expected to be  $8.7 \, \mathrm{times~smallen}$ . The values currently being used are not related to water flux. In the future, source terms will be determined as a function of water per borehole per year. It is expected that they will be converted to concentration as a function of recharge rate [25]. The radionuclides americium and plutonium were not included in this initial preliminary geochemical geophysical model because of lack of a source term.

## Geochemical Properties and Processes

In this section, the limitations of the K sorption model, sorption onto particulates, and effects of temperature are discussed.

## Sorption Model

Using a K\_ for predictive purposes is usually considered to be valid under the assumptions that local chemical equilibrium is attained, the radionuclide is present in trace amounts, the sorption isotherm is linear, and the K, value is spatially and temporally constant and independent of the bulk solution composition. Although the convenience and computational ease of the K approach is beyond dispute, it has had only limited success in modeling observed behavior and its validity as a means of developing reliable predictions of the behavior of contaminants in actual groundwater systems is thus questionable [e.g., 26,27,28,29,30]. The distribution coefficient for a particular radio-uclide is not uniquely dependent on the properties of the porous media but is rather an operational parameter of little or no thermodynamic significance. A K tells nothing about specific chemical reactions occurring in the system, nor about what physical or chemical processes control the reactions. In batch lests, the distribution coefficient is usually determined under a given set of chemical and physical conditions that may or may not be representative of either constant or changing (dynamic) conditions in the field. Limitations and uncertainties that are inherent in the use of the K, approach within the transport framework exist because of geochemical effects, the neterogeneous nature of the stratigraphic units, and the effects of dispersion and advection. Therefore, if the system changes geochemically or geophysically with time, an equilibrium distribution coefficient may not be valid for modeling sorption and transport under the changing or new conditions. A K may be used to place bounds on expected sorption behavior, but it may not be always accurate to use it to model complex chemical processes.

Three examples of the importance for understanding sorption in more detail is () the observed disparity between batch and column results, (2) the sorption of radionuclides as a function of groundwater chemistry, and (3) the transport of radionuclides through fractures.

For neptunium, plutonium, and americium, the distribution coefficients determined from crushed-rock columns are significantly lower than those determined by the batch method [7]. The evidence thus far indicates that actinide sorption may involve one or more time-dependent steps and changes in speciation. If the batch methods are producing relatively larger distribution coefficients than the column experiments for the actinides, we may be overestimating sorption. If these values are used in a transport calculation, we should be at risk of underestimating radionuclide release to the accessible environment.

Second, the groundwater composition controls such factors as the oxidation state, speciation, and solubility of the waste elements and the surface chemistry of the parous media, all of which can affect sorption of radionuclides onto tuff. A recent investigation [31] reported sorption and desorption ratios for cesium, strontium, barium, europium, and tin obtained in batch systems with three different groundwater compositions and three different tuff namples. In a batch system containing CaCl<sub>2</sub> solution, J-13 water, (concentration of Cl = 120 mg L, concentration of Cl = 221 mg L) and a vitric, Topopah Spring Member tuff, the sorption ratio of strontium was an order of magnitude smaller than that observed when pure J-13 water was used One explanation for the decrease in sorption may be the complexation of chloride and strontium reaction competing with the strontium sorption

reaction. This is just one example of how changing the groundwater composition can affect sorption. The limited data reported on the groundwater composition of the vadose zene [31] show the Ca and Cl concentrations at the 91.32-m depth are an order of magnitude greater than the concentrations in pure J-13 water. Therefore, one might expect less sorption in the unsaturated zone than in the laboratory using pure J-13 water. Understanding the geochemical composition of fluid in the unsaturated zone should be given a high priority.

Third, if radionuclides and other undestrable elements of the waste package are transported through fractures, the surface of the fractures may be altered because of precipitation or sorption onto the surface. The radionuclides being transported through the fractures with an altered surface may exhibit different sorption behavior than those observed previously in the laboratory. These changes in sorption may change the overall integrated transport of radionuclides.

To investigate the sorption of radionuclides further and clarify any uncertainties, the following activities should be pursued: (1) assess the validity of using equilibrium distribution coefficients to model sorption of radionuclides (in particular, actinides) on tuffs, (2) examine and define the limits of the applicability of laboratory-measured sorption values to the field situation at Yucca Mountain, (3) evaluate the applicability of using parameter values obtained in the laboratory under saturated conditions in calculations of transport through the unsaturated zone, (4) examine radionuclide sorption under unsaturated conditions, (5) experimentally investigate the sorption of radionuclides by using the geochemical composition of fluid from the unsaturated zone, and (5), if necessary, examine alternative sorption models. These activities should be investigated by using an integrated laboratory, field, and modeling approach.

### Particulates

Leached waste elements could migrate as dissolved species with the groundwater. However, it is also conceivable that particulates moving with the groundwater could strongly sorb various waste species and transport these elements through fractures and open matrix pores. Particulates may be small mineral fragments of the tuffs or natural colloids (e.g., iron hydroxides or ays). Buddemeier and Hunt [32] concluded that transition elements and lanthanide nuclines observed in the field 300 m from a nuclear detonation cavity at the Nevada Test Site are moving by particulate transport. Kerrisk [33] reported the approximate concentration of >0.4-um particulates in J-13 water was 2.7 x 10<sup>-1</sup> g/L. It is clear that the cumulative radionuclide release to the accessible environment may be increased if radionuclides strongly sorb onto particulates that are transported through preferential flow paths. To characterize, quantify, and model particulate transport, data pertaining to the following particulate characteristics should be obtained: (1) concentration, (2) size distribution, (3) composition, (4) adsorption characteristics, (5) agglomeration capture behavior, and (6) source term as relates to particulates.

#### Temperature

Temperature can strongly affect the chemical reactions. Reaction rates and equilibrium sorption ratios maj vary by at least an order of magnitude over the temperature ranges expected within the mountain [34]. Because of the smoothing out of the surface temperature cycles by the intervening layers of material, the model assumes isothermal conditions within the mountain. This is a correct assumption at a distance from the surface (i.e., near the repository). The available values for the K<sub>i</sub>'s (Table I) [7] were all obtained at room temperature, 21°C to 24°C. These values are probably higher [34] than would be found at 34°C, the temperature that would seem to exist

within the mountain. There has been no significant investigation into the effects of temperature on sorption in the far field, although this is clearly an important factor. The experimentally determined values for the sorption ratios can be modified to better approximate those at the actual temperature [35].

## Geophysical Properties and Processes

Several factors need to be included in future geochemical/geophysical models of Yucca Mountain. The stratigraphic model for the transport calculations should include the 5- to 10-degree eastward tilt of the tuffs and explicit faults [6]. In a recent report [16] it was shown that lateral flow caused by the tipped beds occurred under both matrix and fracture flow conditions. Explicit faults, such as Gnost Dance fault, were not included at this time because of the lack of data about fault parameters. The values needed include fault width, porosity, saturation, and hydrologic conductivity or permeability. Even if fracture flow is determined to be insignificant, the tipped beds and faults still need to be modeled because they may provide a very short transport pathway to the water table. If a portion of the flow is diverted around the Tuff of Calico Hills and into a much more permeable fault zone, the groundwater travel time to the accessible environment could be decreased and radionuclide releases could be increased. This scenario should warrant careful consideration in future investigations. The presence of the zeolitic layer and the interaction of this layer with the first two subunits of the Calico Hills thermal mechanical unit also should be more fully represented.

#### CONCLUSIONS AND RECOMMENDATIONS

As a precursor to modeling the transport of radionuclides at the potential repository, a comprehensive geochemical geophysical model must be compiled. In this report, a geochemical geophysical model, which incorporates the relevant stratigraphic, petrologic, hydrologic, geochemical, and material data is discussed. This model provides a referenced and up-to-date foundation on which to base radionuclide transport calculations.

The following important factors in model development are observed:

- (1) Many of the stratigraphic units do not have associated  $K_d$  values obtained from experiments performed on field samples.
- (2) The sorption ratio data exhibit large amounts of spatial nonuniformity and associated uncertainties. For example, the K value for  $^{9}$ Tc in the RSw2 stratigraphic unit is 4 times larger than the next largest value.
- (3) There has been no adequate investigation into the effects of temperature on sorption.
- (4) For the actinides, the batch sorption method produced a larger sorption ratio than did the circulating-column and crushed-rock experiments.
- (5) Investigations concerning the natural groundwater flow in the unsaturated zone are in the preliminary stages.
- (6) Values for the dispersion coefficients have not been measured.
- (7) Information is scarce concerning the source term for the radionuclides known to exist in the waste package. For two of the radionuclides, technetium and uranium, a source term is available.

The following principal conclusion was reached from compiling this preliminary geochemical geophysical model:

More data are needed before the geochemical geophysical model of Yucca Mountain can be regarded as a suitable base for multidimensional flow and transport predictive simulations.

The following recommendations are made for future studies and data acquisition to more fully characterize the site:

- (1) Unless data can be inferred with an adequate degree of confidence, more geochemical scription and material properties data should be gathered. In some cases, data exist within one layer but none exist within the next layer.
- (2) There is a strong need for some type of data analy is, such as kriging, on the parameters involved with characterizing the geologic medium. For example, the saturation, porosity, and bulk density data could perhaps be extrapolated to locations away from the drill holes, and estimates of error could be assigned to the parameter values.
- (3) Experimental error estimates should be provided by those obtaining the data.
- (4) More specific geochemical effects should be investigated, such as the effects of groundwater chemistry and temperature on sorption and alternative sorption models should be examined.
- (5) The validity of using the distribution coefficient to model sorption at Yucca Mountain should be evaluated.
- (6) Laboratory and field experiments to investigate sorption under unsaturated conditions may have to be performed.
- (7) Sorption of radionuclides onto particulates may be an important process and the presence of particulates should be investigated.
- (8) Tipped material layers and explicit faults need to be included in the stratigraphic model used in transport calculations.
- (9) A better understanding of the natural groundwater flow in each of the stratigraphic units is needed.
- (10) Mechanical dispersion and the dispersivity of the welded and nonwelded tuffs need to be quantified and better examined.
- (11) Laboratory investigations should be integrated with the field and modeling investigations.

Based on these observations and recommendations, iterative modeling, professional judgement, and programmatic requirements will have to be applied to assess future research plans which will be german? to calculating the limited release of radionuclides over 10,000 Y.

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Table I [5]

AVAILABLE, (A), AND ESTIMATED, (E),

K<sub>d</sub>VALUES FOR YUCCA MOUNTAIN TUFFS

	Te		U		Pu		Am	
	(cm³/	<u>g)</u>	( cm <sup>3</sup>	/g)	(cm <sup>3</sup> /)	<u>z)</u>	(cm³=	g)
Unit	(A)	(E)	(A)	(E)	(A)	(E)	(A)	(E)
TCw		0.346		2.84		165		3860
PTn	0.006		5.90		4500		885000	
TSw1	0.159		0.75		195		3 <b>6</b> 90	
TSW2	0.72			2.84	220			3860
TSw3	0.00		0.00		363		1110	
CHn 1v	0.04		0.00		290		1760	
CHn 1z	0 0098		5.33		59.8		3330	
CHn2		0.0098	12.0			59.8		3330
CHn3		0.0098		6.75		59.8		3330
PPw		0.346	2.4		51.0		4200	
CFUi	0.181		4.03		298		2900	
BF₩		0.346	4.98			165		3860
CFMn 1		0.0098		6.75		59.8		3330
CFMn2		0.0098		6.75		59.8		3330
CFMn3		0.0098	4.35			59.8		3330
TRw		0.346	0.5			165		3860

TABLE II

MATERIAL PROPERTIES OF STRATIGRAPHIC UNITS

Unit	Saturation [21]	Porosity [12]	Bulk Density [12] ρ(g cm³)
TCw	0.8614	NA	2.25
PTn	0.8241	NA	1,42
TSw1	0.8153	0.11681	2.17
TSu2	0.8857	0.11681	2.26
TSw3	o.7588	0.11681	2.30
CHn 1 v	0.8598	C.35405	1.53
CHn1z	0.8896	0.30636	1.59
CHn2	0.9144	0.39636	1.78
CHn3	0.9401	0.30636	1.48
P₽₩	0.8474	0.25274	1.88
CFUn	0.9203	0.32393	1.64
BFw	0.8706	0.23909	1.98
CFMn 1	0.9291	0.25572	1 . 84
CFMN2	0.9803	0.25572	1.8
CFMN3	0.9472	0.25572	1.75
TR₩	0.0974	0 20383	2.08

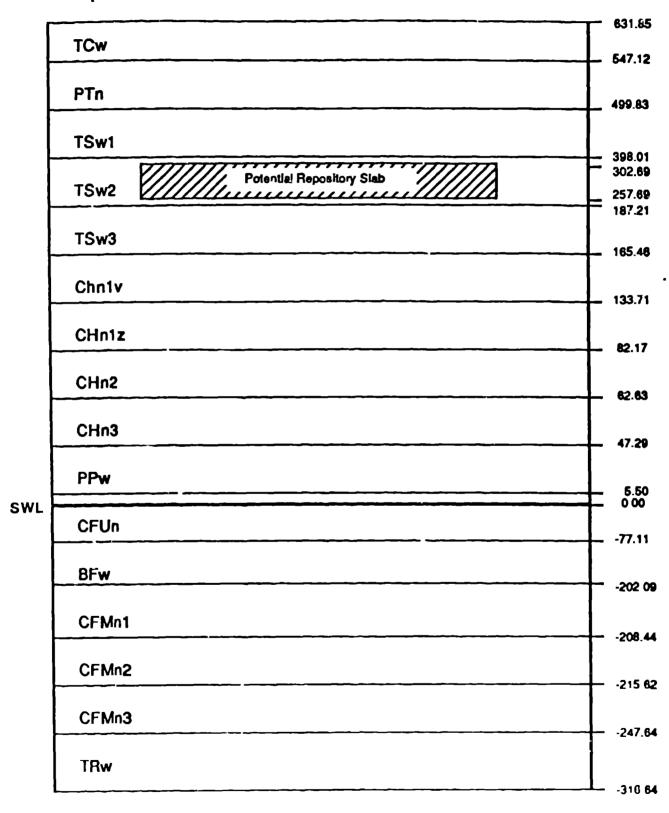


Figure 1. From Eq. stratigraphy for two a Magnifican conditions and the  $\gamma$